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Hamiltonian walk on different deterministic fractals and stochasticity

Mohammad-Ali Jafarizadeh[1,2] and Kamal Seyed-Yagoobi[1]
[1] Department of Physics, University of Tabriz, Tabriz, Iran
[2] Institute for Studies in Theoretical Physics and Mathematics, Tehran, Iran

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Abstract : We introduce mixed fractals and give a prescription for calculating their fractal dimensions Using Perron-Frobenius theorem about stochastic matrices, we estimate lower and upper limits of critical exponent ν for Hamiltonian self-avoiding walks and Hamiltonian self trail We show that in almost all cases $1/\nu$ equals the fractal dimension of the fractals.

Keywords : Hamiltonian walk, fractal dimensions, stochasticity

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1. Introduction

Lattice models, such as random walk, self avoiding walk and self trail have been the focus of much attention. They provide models for polymer chains in different regimes, also models for diffusion and conduction in random media. From the statistical mechanics viewpoint, they serve as the generic examples to analyze scaling and fractal properties [1,2]. In zero temperature limit, one comes across a walk called Hamiltonian walk when studying collapsed polymer chains [3,4].

In all these walks, the exponent ν is defined according to the following equation [5]

$$\langle N(R)\rangle \sim R^{1/\nu},$$

where $<N>$ and R are the mean number of steps and fractal size respectively.

In Section 2, after introducing d-simplex fractal, we calculate the fractal dimension by coding its subfractals according to the partition of $(b-1)$, (b is decimation number), into $(d+1)$ non-negative integers and by using Bose-Einstein statistics. Then we define various new fractals, called mixed fractals, and derive a general expression for their fractal dimensions in terms of fractal dimensions of their components. Here we give two examples in order to illustrate mixed fractals : (a) hypercubic fractal, a d-dimensional generalization of Sierpinski carpet [6], and (b) prism fractal. Then we calculate their fractal dimension from the general prescription of fractal dimension of mixed fractals proposed by the authors. In Section 3, we define the required possible walks and corresponding generating functions. Then in Section 4, we explain the stochastic property of the matrix appearing in the recursion relations of the mean number of steps. Using Perron-Frobenius theorem, we can then estimate upper and lower bounds of the exponent v for the Hamiltonian self avoiding walk and self trail respectively. We prove that in most cases, $1/v$ equals the fractal dimension of the fractals. The paper is concluded with a brief discussion in Section 5. The proof of the positivity of the matrix appearing in the recursion relations of the mean number of steps is included as an appendix.

2. Fractals

2.1. (d + 1) simplex fractals :

$d + 1$ simplex fractal is generalization of a 2-dimensional Sierpinski gasket [6] to d-dimensions such that its subfractals are $(d + 1)$ simplices or d-dimensional polyhedra.

To obtain a fractal with decimation number b, we choose a $(d + 1)$ simplex and divide all the links (that is the lines connecting the sites) into b parts and then draw all possible d-dimensional hyper-planes through the links parallel to the transverse d-simplices Next, having omitted every other inner polyhedra, we repeat it for the remaining simplices or for the subfractals of next higher order. This way through $(d + 1)$ simplex fractals are constructed. To calculate fractal dimension, we label subfractals of order $(l + 1)$ in terms of partition of $(b - 1)$ into $(d + 1)$ positive integers $\lambda_1, \lambda_2, \cdots, \lambda_{d+1}$. Each partition represents a subfractal of order l and λ shows the distance of the corresponding subfractal from d-dimensional hyper-planes which construct the $(d + 1)$ simplex. As an illustrating example, the method of labelling a Sierpinski gasket with decimation number $b = 3$ is shown in Figure 1.

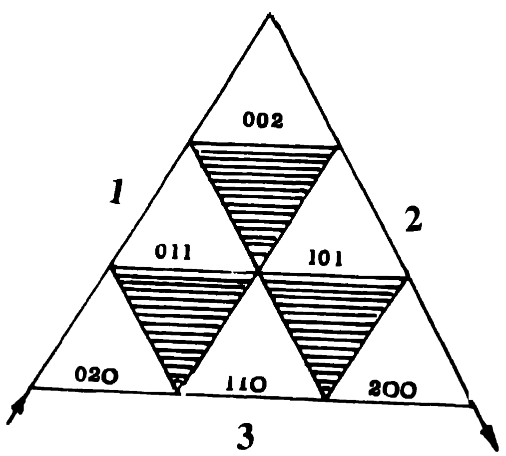

Figure 1. A Sierpinski gasket with decimation number $b = 3$.

Obviously the number of all possible partitions is equal to the distribution of $(b-1)$ objects amongst $(d+1)$ boxes, which is the same as the Bose-Einstein distribution of $(b-1)$ identical bosons in $(d+1)$ quantum states. This is equal to

$$c = \frac{(d+b-1)!}{(b-1)!\,d!}. \tag{1}$$

As is well known, the fractal dimension d_F of a self similar object is defined according to [6]

$$\left(N^r\right)^{d_F} = 1, \tag{2}$$

where N is the number of similar objects, up to translation and rotation, and here is equal to the number of subfractals of order r. In eq. (2), $N = c^N$ and $r = b^{-N}$. Therefore $d_F = \ln c/\ln b$, or

$$d_F = \frac{1}{(\ln b)} \ln\left[\frac{(b+d-1)!}{(b-1)!\,d!}\right]. \tag{3}$$

2.2. *d-Dimensional hypercubic fractals :*

A d-dimensional hypercubic fractal with an odd decimation number b, is constructed by dividing the links of a hypercube in d-dimensions into b sections, then passing through the intersecting points d-dimensional hypersurfaces perpendicular to the links. Next, having omitted every other sub-hypercubes, apply the same method to the remaining sub-hypercubes. In Figure 2, we illustrate this for $d = 2$ and $b = 3$.

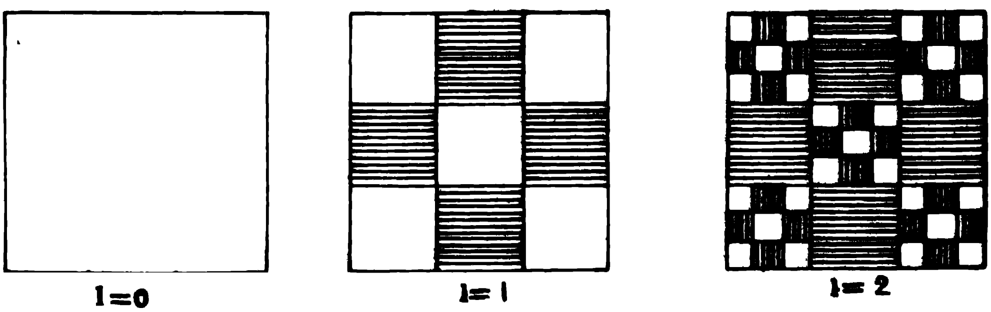

Figure 2. A two dimensional 'hypercube' with $b = 3$, for different values of l.

To calculate the corresponding fractal dimension d_F, we first note that the number of subfractals is $(b^2+1)/2$. Therefore, following the procedure mentioned for n-simplices, one can easily calculate d_F as

$$d_F = \ln\left(\left[b^2/2\right] + 1\right) / \ln b, \tag{4}$$

where the symbol [] stands for the greatest integer.

2.3. Mixed fractals :

As we know, deterministic fractals are constructed by repeatedly decimating a geometric object F, where according to some rule, at each step, one keeps a number of the decimated ones as subfractals (F^{N0}) and omits the remaining (F^0).

To construct mixed fractals, first we take the Cartesian product of two geometrical objects of some fractals as our geometric object, then do the decimation in each of them. For the subfractals thus obtained, we take the product of those chosen as subfractals in usual procedure of construction of fractals and also the Cartesian product of the omitted decimated ones, if they are similar to the previously obtained fractals. For the fractal dimension of mixed fractal, we note that number of sub-mixed fractals is equal to some number C :

$$C = b^{\left(d_{F1}^{N0} + d_{F2}^{N0}\right)} + b^{\left(d_{F1}^{0} + d_{F2}^{0}\right)}. \tag{5}$$

So, we can conclude that the fractal dimension d_F of the mixed fractal is

$$d_F = \frac{1}{\ln b} \ln \left[b^{\left(d_{F1}^{N0} + d_{F2}^{N0}\right)} + b^{\left(d_{F1}^{0} + d_{F2}^{0}\right)} \right], \tag{6}$$

where b is the decimation number, d_{F1}^{0} (or d_{F2}^{0}) and d_{F1}^{N0} (or d_{F2}^{N0}) are the omitted and non-omitted fractal dimensions of the individual fractals F_1 (or F_2) respectively. Also note that had we not kept F_1^0 and F_2^0 in eq. (6), or in other words, had we just taken the Cartesian product of the fractals, we could have arrived at the conclusion that $d_F = d_{F1} + d_{F2}$ [8]: The above prescription can simply be generalized to the case of many fractals. As a newly obtained fractal, we can keep those which are constructed by even number of omitted objects. The fractal dimension is similarly given by

$$d_F = \ln \left[\sum_{(c_1 \cdots c_N) \in (0, N0)} b^{d_{F1}^{(c_1)} + \cdots + d_{F_N}^{(c_N)}} \right], \tag{7}$$

where for any set of indices $\{c_1, \cdots, c_N\}$, the number of omitted $d_{F1}^{(c_1)}, \cdots, d_{F_N}^{(c_N)}$ in the exponent is even.

To clarify the matter further, two points are in order. *First*, we note that the carpet fractal is itself a product of two Cantor sets. The fractal dimension of Sierpinski carpet given by eq. (4) easily follows from eq. (6) for an odd b

$$d_F = \frac{1}{\ln b} \ln b^{\left(d_{F_1}^{N0} + d_{F_2}^{N0}\right)} \tag{8}$$

d-Dimensional hypercubic fractals are mixed fractals consisting of d Cantor sets. According to eq. (7), one can easily verify the corresponding fractal dimension for odd b to be

$$d_F = \frac{1}{\ln b} \ln \left[\sum_{l=0}^{[d/2]} (b + 1/2)^{d-2l} (b - 1/2)^{2l} \right]. \tag{9}$$

Second, as Figure 3 shows, the product of two fractals, one a Sierpinski gasket (as the base) and the other a Cantor set (as the height) is a prism fractal

$$d_F = \frac{1}{\ln b} \ln\left(\frac{b(b^2+1)}{2}\right). \tag{10}$$

3. Generating functions

3.1. Self-avoiding Hamiltonian walk :

To study self avoiding Hamiltonian walk in a deterministic fractal with decimation number b, we will need to calculate $< N_M >$, *i.e.* the mean number of steps in a subfractal of order M. Therefore, $< N >$ can be calculated by letting $M \to \infty$. To proceed, we choose the following definition for our walks [4] :

$P_{kl}^M(n)$: the number of self-avoiding walks with n steps in which a walker enters the subfractal of order M at one vertex and exits at another with (i) visiting k vertices ($k = 0, 1, \cdots$) and (ii) re-entering l times ($l = 0, 1, 2, \cdots$); without violating self avoidness.

The generating functions of step l are defined as

$$G_{kl}^M(z) = \sum_{n=0} P_{kl}^M(n) z^n, \qquad (k = 0, 1, 2, \cdots) \text{ and } |z| \le l. \tag{11}$$

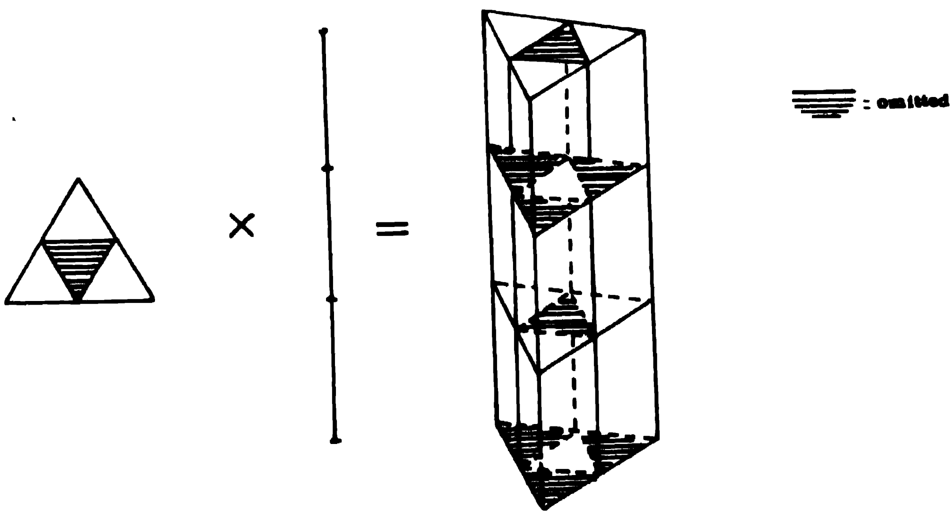

Figure 3. A mixed fractal as a product of two fractals.

Generating functions satisfy the following recursion relation

$$G'_{kl}(z) = F_{kl}\left[G^M(z)\right], \tag{12}$$

where F_{kl} are homogeneous polynomials of degree d_{kl}, that is the number of subfractals that the walker can visit without violating self-avoidness. We note too that the coefficients of the polynomial are positive integers. This is due to the fact that the walker is obliged to visit every subfractal.

One can write $< N_{kl} >$ in terms of the generating functions (11) :

$$\langle N_{kl} \rangle = \lim_{M\to\infty} \left[\sum_{n=0}^{\infty} \left(n\, P_{kl}^{M}(n) \right) \Big/ \left(\sum_{n=0}^{\infty} P_{kl}^{M}(n) \right) \right] = \lim_{\substack{M\to\infty \\ z\to 1^-}} \left[\frac{1}{G_{kl}^{M}} \frac{dG_{kl}^{M}}{dz} \right]$$

$$(k,l = 0, 1, 2, \cdots). \tag{13}$$

To find ν, we use the real space renormalization group technique. This means that in order to calculate $< N >$, we must linearalize the recursion relation (12) around the fixed point. Therefore

$$N'_{kl} G_{kl} = \sum_{p,q} \frac{\partial F_{kl}}{\partial G_{pq}} G_{pq} N_{pq}, \qquad (k,l = 0, 1, 2, \cdots) \tag{14}$$

or in the matrix form

$$N'_{kl} = \sum_{p,q} a_{kl,\,pq} N_{pq}, \tag{15}$$

where
$$a_{kl,\,pq} = \frac{1}{G_{kl}} \frac{\partial F_{kl}}{\partial G_{pq}} G_{pq}. \tag{16}$$

ν is calculated by

$$1/\nu = \frac{\ln \lambda_{\max}}{\ln b} \tag{17}$$

where $\lambda_{\max}$ is the largest eigenvalue of the matrix defined by (16).

3.2. Hamiltonian self-trail :

Hamiltonian self-trail is a kind of walk where a walker is obliged to visit every subfractal and can visit every site as many times as it wishes but is not allowed to go through a given link more than once [7].

In self trail case, in addition to the above-mentioned walk, one needs to define that kind of a walk where entering and re-exiting from the same vertex is permitted. So we define $P_{kl_r}^{M}$, where r is the number of vertices through which entering and re-exiting from the same point have occurred. The rest of the procedure follows the self-avoiding case, with the exception that here the walker will definitely visit every subfractal without violating self-trailness. Here, therefore, the exponent $1/\nu$ is nothing but the fractal dimension of the fractal lattice.

4. Stochasticity

Our recursion relations for generating functions are homogeneous polynomials of degree d, *i.e.* the number of subfractals that the walker can visit without violating self avoidness, with positive integers. Based on physical conditions, the values of generating functions at the corresponding fixed points are positive. Therefore, the corresponding matrix elements $a_{kl,pq}$ are all positive and non-zero. The reason why none of the elements cannot be zero, is given in the appendix. This shows that the matrix is primitive. By definition, a matrix is primitive if $a^k > 0$, for all $k \geq 1$ [9]. According to the Perron-Frobenius theorem for primitive matrices ([9], page 3), there exists and eigenvalue λ_{max} such that (we quote) :

(a) λ_{max} real, > 0.

(b) with λ_{max} can be associated strictly positive left and right eigenvectors.

(c) $\lambda_{max} > |\lambda|$ for any eigenvalue $\lambda \neq \lambda_{max}$.

(d) the eigenvectors associated with λ_{max} are unique to constant multiples.

(e) If $0 \leq B \leq A$ and μ is an eigenvalue of B, then $|\mu| \leq \lambda_{max}$. Moreover, $|\mu| = \lambda_{max}$ implies $A = B$.

(f) r is a simple root of the characteristic equation of A.

According to the corollary of the theorem ([9], page 8) we have

$$\min \sum_{j=1}^{n} a_{ij} \leq r \leq \max \sum_{j=1}^{n} a_{ij}, \tag{18}$$

with equality on either side implying equality throughout (that is r can only be equal to the maximal or minimal row sum if all row sums are equal). A similar proposition holds for column sums (end of quotation.)

We also note that our matrix a_{ij} is a Perron matrix. An $n \times n$ matrix $A = \{a_{ij}\}$ is said to be Perron if $f(A) > 0$ for some polynomial f with real coefficients ([9], page 48). Here we have $f(A) = A$. Therefore (a), (b), (f) and the corollary already quoted for primitive matrices, also hold for Perron matrices.

The walker can visit every subfractal in any dimension if it is self-trail and in self-avoid it can visit all subfractals of almost all fractals of more than two dimensions. Therefore, all functions F_{kl} in (4) are homogeneous polynomials of degree equal to the number of subfractals in decimation process. Hence due to the theorem of Euler on homogeneous polynomials, we can conclude that

$$\sum_{j=1}^{n} a_{ij} = C, \qquad \text{for all } i = 1, \cdots, n \tag{19}$$

where C is the number of subfractals. Therefore r defined in (f) is equal to C, so one can write

$$a_{ij} = C\, p_{ij}. \tag{20}$$

P_{ij} are matrix elements of a stochastic matrix where all p_{ij} are non-negative [8]. Here, obviously, they are positive and satisfy

$$\sum_{j=1}^{n} P_{ij} = 1.$$

Therefore, $r = \lambda_{max} = C =$ number of subfractals.

Then according to (8)

$$\frac{1}{\nu} = \frac{\ln \lambda_{max}}{\ln b} = \frac{\ln C}{\ln b} = d_F.$$

Hence $1/\nu$ for the Hamiltonian self trail in any dimension and for the Hamiltonian self avoid in more than two dimensions, is equal to the fractal dimension of the fractals.

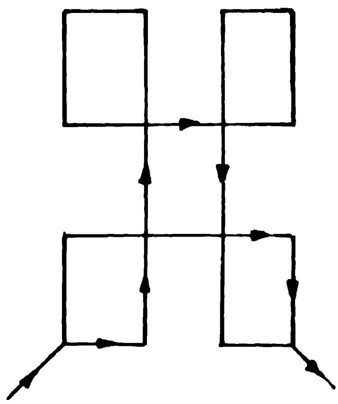

Figure 4. A Sierpinski carpet

But for the case of self-avoiding walk in 2 dimensions such as the Sierpinski carpet, Figure 4, there is a possibility that the walker cannot visit subfractals in the corners due to self avoid constraint. In this case

$\min \sum_{j=1}^{n} a_{ij} \doteq$ the minimum number of subfractals which the walker can visit without violating constraint of self-avoidness,

and $\max \sum_{j=1}^{n} a_{ij} =$ the maximum number of subfractals which the walker can visit without violating constraint of self-avoidness.

Therefore, $1/\nu$ satisfies the following inequality

$$\frac{\ln \text{ (max. num. of walks)}}{\ln b} < \frac{1}{\nu} < d_F.$$

In Sierpinski carpet we have

$$\frac{\ln\left(\left[b^2/2\right] - 1\right)}{\ln b} < \frac{1}{\nu} < d_F = \frac{\ln\left(\left[b^2/2\right] + 1\right)}{\ln b}. \tag{21}$$

As can be easily verified, the fractal dimension calculated in [5] satisfies the inequality (21).

5. Conclusion

In Ref. [4], the authors have proved directly that the exponent v of self avoiding Hamiltonian walk for n-simplex fractal is proportional to the inverse of its fractal dimension.

Here, using Perron-Frobeneus theorem on positive matrices, specially the stochastic ones, we have proved that the exponent $1/v$ for the Hamiltonian walk and for Hamiltonian trails in most of the fractals equals their fractal dimension. Also for the self-avoiding Hamiltonian walk for the two dimensional Sierpinski carpet, the lower and upper limits of $1/v$ have been determined.

Acknowledgments

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Appendix

Here, we prove that the matrix elements defined by

$$a_{k1,pq} = \frac{1}{G_{k1}} \frac{\partial F_{k1}}{\partial G_{pq}} G_{pq},$$

are all non-negative for n-simplex fractals with an arbitrary decimation number. This can be proved for other fractals similarly, but it is rather complicated.

Let us define

$$A = \sum_{l=1}^{[V/2]-1} \sum_{k=0}^{V-2l-1} \alpha_{k,1} G_{k,1}$$

and $$B = \sum_{l=1}^{[V/2]-1} \sum_{k=0}^{V-2l-1} \alpha_{k,l}\, G_{k+1,l}$$

where V is the number of vertices. Then, using the symmetry of d-simplex fractals, the recursion relation takes the following form at the fixed point

$$G_{kl} = {}^{*}F_{kl} = A^{(V-2l-k)} B^{k} F_{l}, \qquad l = 0, 1, \cdots . \tag{A-1}$$

Now, multiplying both sides by α_{kl} and summing over l and k, we get

$$A = A \sum_{l} \left(\sum_{k} \alpha_{kl} A^{V-2l-k} B^{k} \right) F_{l}. \tag{A-2}$$

Since just the non-negative values of G_{kl} at the fixed point are physically acceptable, therefore A is definitely a positive quantity. Since the coefficient α_{kl} of (A-2) is positive and because $G_{kl} \neq 0$ for all k and l, as again this would not be a physically acceptable fixed point, therefore we can drop off A on both sides and get .

$$1 = \sum \left(\sum \alpha_{kl} A^{V-2l-k} B^{k} \right) F_{l}. \tag{A-3}$$

Similarly by multiplying both sides of the equation by $\alpha_{k+1,l}$ and summing over k and l, we can arrive at the same equation as above. So we conclude that the recursion relations are not all independent. This means that the fixed point is not an isolated point, but at least, a one dimensional manifold. Therefore, one can choose it as a fixed $G_{kl} \neq 0$ for all k and l.

Furthermore, all of the generating functions appear on the right hand side of $F_{kl} = A^{(V-2l-k)} B^{k} F_{l}$. Hence $\partial F_{kl}/\partial G_{pq} \neq 0$ for all values of (k, l) and (p, q). Therefore the positivity of $a_{kl,\,pq}$ follows. For other fractals similar to the d-simplex case, recursion relation for $G'_{k+1,\,l}$ can be obtained from $G'_{k,\,l}$, simply by replacing $G_{k+1,l}$ with G's in the subfractals located at the vertices of the fractal, provided that it has entrance from and exit to the outside. Therefore, the fixed point will be a manifold instead of an isolated point. So G_{kl} could be chosen all nonzero at the fixed point, and therefore positivity of $a_{kl,\,pq}$ follows similar to the d-simplex fractals. If $k = 0$ is the only possibility, then the recursion relation can converge to an isolated point but then G_{l0} will appear definitely on the righthand side of all the recursion relations (13), therefore all G_{l0} would be nonzero, otherwise G_{l0} itself would be zero, which is not physically acceptable, as we have already mentioned.